

Author index to volume 213

- Abramczyk, H., see Kolodziejski, M. 213 (1996) 341
Adamowicz, L., see Sobolewski, A.L. 213 (1996) 193
André, J.-M., see Jacquemin, D. 213 (1996) 217
Andrews, D.L. and I.D. Hands, Second harmonic generation in partially ordered media and at interfaces: analysis of dynamical and orientational factors 213 (1996) 277

Belchior, J.C. and J.P. Braga, A critical analysis of the two-dimensional atom ellipsoid model to study rotational collisions 213 (1996) 303
Belikov, A.E., R.G. Sharafutdinov and A.V. Storozhev, Rotational relaxation of nitrogen in helium 213 (1996) 319
Bernardes, E.S., Y.M.M. Hornos and J.E.M. Hornos, Dynamical symmetry in the vibrational overtone spectrum of monofluoroacetylene (HCCF) 213 (1996) 17
Bertault, M., see Even, J. 213 (1996) 357
Bieser, G., see Lossau, H. 213 (1996) 1
Borchert, I., see Ruth, C. 213 (1996) 454
Braga, J.P., see Belchior, J.C. 213 (1996) 303
Braga, M., Correlation effects in the long-range coupling between acetylenic π -electrons in a series of α,ω -diethynyl[n]staffanes ($n = 1-5$) 213 (1996) 159
Byrd, E.F.C., see Chesnut, D.B. 213 (1996) 153

Cannistraro, S., see Lamanna, R. 213 (1996) 95
Cao, H., see Xie, X. 213 (1996) 133
Champagne, B., see Jacquemin, D. 213 (1996) 217
Chesnut, D.B. and E.F.C. Byrd, The use of locally dense basis sets in correlated NMR chemical shielding calculations 213 (1996) 153
Clark, B.K., J.M. Standard, Z.J. Smolinski, D.P. Ripp and J.R. Fleming, Optically pumped laser emission in K_2 involving rovibrational levels near the $B^1\Pi_u$ state dissociation limit 213 (1996) 229
Comes, F.J., see Lock, M. 213 (1996) 385
Consolati, G. and F. Quasso, Positronium dynamics in aqueous solutions of ionic surfactants 213 (1996) 449
Cooksy, A.L., see Wang, H. 213 (1996) 139
Cormack, A.J., A.J. Yench, R.J. Donovan, K.P. Lawley, A. Hopkirk and G.C. King, High-resolution threshold photoelectron spectroscopy of molecular fluorine 213 (1996) 439
Czerwiński, M. and J. Dąbrowski, Spin-spin interactions in the reduced $[Fe_6S_6]^{5+}$ cluster 213 (1996) 45

Dąbrowski, J., see Czerwiński, M. 213 (1996) 45
Dashevskaya, E.I., see Rosenblum, I. 213 (1996) 243

- Délugeard, Y., see Even, J. 213 (1996) 357
Donovan, R.J., see Cormack, A.J. 213 (1996) 439
Duang, W., see Xie, X. 213 (1996) 133
Durig, J.R., S. Shen, W. Zhao and L. Zhou, Conformational studies of cyclopropylcarbonyl fluoride from temperature dependent FT-IR spectra of xenon solutions 213 (1996) 165
Durig, J.R., Y. Li and Y. Jin, Conformational studies of propenoyl chloride in liquid xenon from temperature dependent FT-IR spectra 213 (1996) 181

Engdahl, A. and B. Nelander, IR induced isomerisation of HDO complexes: a method for the observation of FIR spectra of matrix isolated water complexes 213 (1996) 333
Engkvist, O. and G. Karlström, A method to calculate the probability distribution for systems with large energy barriers 213 (1996) 63
Eschrich, I., see Ruth, C. 213 (1996) 454
Even, J., M. Bertault, A. Girard and Y. Délugeard, Influence of pressure on the ferroelectric phase transition in a symmetrical polymerizable diacetylene crystal DNP 213 (1996) 357

Fleming, J.R., see Clark, B.K. 213 (1996) 229

Gericke, K.-H., see Lock, M. 213 (1996) 385
Girard, A., see Even, J. 213 (1996) 357
Goto, T., see Oeda, Y. 213 (1996) 421
Gründel, M., see Ruth, C. 213 (1996) 454
Grycuk, T., see Roston, G.D. 213 (1996) 365

Habdas, P., see Paluch, M. 213 (1996) 483
Hands, I.D., see Andrews, D.L. 213 (1996) 277
Heinecke, R., see Lossau, H. 213 (1996) 1
Helmi, M.S., see Roston, G.D. 213 (1996) 365
Hikida, T., see Matsushita, Y. 213 (1996) 413
Hopkirk, A., see Cormack, A.J. 213 (1996) 439
Hornos, J.E.M., see Bernardes, E.S. 213 (1996) 17
Hornos, Y.M.M., see Bernardes, E.S. 213 (1996) 17
Huber, H., see Welker, M. 213 (1996) 253

Ivanov, V.S. and V.B. Sovkov, An IPA procedure for bound-continuum diatomic transition intensities 213 (1996) 295

Jacquemin, D., B. Champagne, J.-M. André and B. Kirtman, Exploratory Pariser-Parr-Pople investigation of the static first hyperpolarizability of polymethineimine chains 213 (1996) 217
Jin, Y., see Durig, J.R. 213 (1996) 181
Jonsson, T., see Lossau, H. 213 (1996) 1

Karlström, G., see Engkvist, O. 213 (1996) 63
Keith, T.A., Calculation of magnetizabilities using GIAO current density distributions 213 (1996) 123
King, G.C., see Cormack, A.J. 213 (1996) 439
Kirtman, B., see Jacquemin, D. 213 (1996) 217
Knast, K., Analysis of polarization effects in time-dependent Rayleigh light scattering by optically active molecules 213 (1996) 465

- Kohlmeyer, A., W. Witschel and E. Spohr, Molecular dynamics simulations of water/metal and water/vacuum interfaces with a polarizable water model 213 (1996) 211
- Kolodziejewski, M., G. Waliszewska and H. Abramczyk, Vibrational dephasing in bromocyclohexane: how to separate contributions from different mechanisms 213 (1996) 341
- Kompa, C., see Lossau, H. 213 (1996) 1
- Kummer, A., see Lossau, H. 213 (1996) 1
- Lamanna, R. and S. Cannistraro, Effect of ethanol addition upon the structure and the cooperativity of the water H bond network 213 (1996) 95
- Lawley, K.P., see Cormack, A.J. 213 (1996) 439
- Levine, R.D., see Raz, T. 213 (1996) 263
- Li, Y., see Durig, J.R. 213 (1996) 181
- Lock, M., K.-H. Gericke and F.J. Comes, Photodissociation dynamics of $\text{HN}_3(\text{DN}_3) + h\nu \rightarrow \text{H(D)} + \text{N}_3$ 213 (1996) 385
- Lossau, H., A. Kummer, R. Heinecke, F. Pöllinger-Dammer, C. Kompa, G. Bieser, T. Jonsson, C.M. Silva, M.M. Yang, D.C. Youvan and M.E. Michel-Beyerle, Time-resolved spectroscopy of wild-type and mutant Green Fluorescent Proteins reveals excited state deprotonation consistent with fluorophore-protein interactions 213 (1996) 1
- MacKenzie, V.J., see Sinha, H.K. 213 (1996) 397
- Martin, J.-P., see Porshnev, P.I. 213 (1996) 111
- Matsui, A.H., see Oeda, Y. 213 (1996) 421
- Matsushima, Y., see Oeda, Y. 213 (1996) 421
- Matsushita, Y., Y. Yamaguchi and T. Hikida, The photochemical reaction of excited acetophenone and benzaldehyde in the gas phase 213 (1996) 413
- Michel-Beyerle, M.E., see Lossau, H. 213 (1996) 1
- Michinomae, M., see Oeda, Y. 213 (1996) 421
- Mizuno, K., see Oeda, Y. 213 (1996) 421
- Motohashi, K., H. Soshi, M. Ukai and S. Tsurubuchi, Dissociative excitation of CH_4 by electron impact: Emission cross sections for the fragment species 213 (1996) 369
- Naumkin, F.Y., The ArClF Van der Waals complex as an example of how atoms inside a molecule interact with those outside 213 (1996) 33
- Nelander, B., see Engdahl, A. 213 (1996) 333
- Nikitin, E.E., see Rosenblum, I. 213 (1996) 243
- Nishi, O., see Oeda, Y. 213 (1996) 421
- Oeda, Y., O. Nishi, Y. Matsushima, K. Mizuno, A.H. Matsui, M. Michinomae, M. Takeshima and T. Goto, Exciton scattering, k selection rule, exciton bandwidth in pyrene microcrystallites, and lattice relaxation energy for the origin of V luminescence 213 (1996) 421
- Oref, I., see Rosenblum, I. 213 (1996) 243
- Paluch, M., P. Habdas, S.J. Rzoska and T. Schimpel, Electric permittivity in the one- and two-phase region of 1-nitropropane-hexadecane near-critical solution 213 (1996) 483
- Penzkofer, A., see Reindl, S. 213 (1996) 429
- Perrin, M.-Y., see Porshnev, P.I. 213 (1996) 111
- Pöllinger-Dammer, F., see Lossau, H. 213 (1996) 1

- Porshnev, P.I., H.L. Wallaart, M.-Y. Perrin and J.-P. Martin, Modeling of optical pumping experiments in CO. I. Time-resolved experiments 213 (1996) 111
- Quasso, F., see Consolati, G. 213 (1996) 449
- Raz, T. and R.D. Levine, Fast translational thermalization of extreme disequilibrium induced by cluster impact 213 (1996) 263
- Reindl, S. and A. Penzkofer, Triplet quantum yield determination by picosecond laser double-pulse fluorescence excitation 213 (1996) 429
- Ripp, D.P., see Clark, B.K. 213 (1996) 229
- Rode, B.M., see Vizoso, S. 213 (1996) 77
- Rosenblum, I., E.I. Dashevskaya, E.E. Nikitin and I. Oref, On the sampling of microcanonical distribution for rotating triatomic molecules 213 (1996) 243
- Roston, G.D., M.S. Helmi and T. Grycuk, Interatomic potentials for $X0^+$ and B^31 states of intercombination cadmium line 326.1 nm broadened by Ar pressure 213 (1996) 365
- Ruth, C., M. Gründel, I. Eschrich, L. Ziegeler and I. Borchert, Influence of the molecular environment on the hyperfine interaction of ^{111}Cd ions in gaseous radioactive indium halides 213 (1996) 454
- Rzoska, S.J., see Paluch, M. 213 (1996) 483
- Sansón, J.A., see Tolosa, S. 213 (1996) 203
- Schimpel, T., see Paluch, M. 213 (1996) 483
- Sharafutdinov, R.G., see Belikov, A.E. 213 (1996) 319
- Shen, S., see Durig, J.R. 213 (1996) 165
- Silva, C.M., see Lossau, H. 213 (1996) 1
- Sinha, H.K., V.J. MacKenzie and R.P. Steer, Laser-induced fluorescence excitation spectroscopy of jet-cooled tropolone-carbon monoxide van der Waals complexes 213 (1996) 397
- Smolinski, Z.J., see Clark, B.K. 213 (1996) 229
- Sobolewski, A.L. and L. Adamowicz, An ab initio study of the potential energy surface in the S_1 state of 2-hydroxypyridine 213 (1996) 193
- Solca, J., see Welker, M. 213 (1996) 253
- Soshi, H., see Motohashi, K. 213 (1996) 369
- Sovkov, V.B., see Ivanov, V.S. 213 (1996) 295
- Spohr, E., see Kohlmeyer, A. 213 (1996) 211
- Standard, J.M., see Clark, B.K. 213 (1996) 229
- Steer, R.P., see Sinha, H.K. 213 (1996) 397
- Steinebrunner, G., see Welker, M. 213 (1996) 253
- Storozhev, A.V., A new method of calculating exponential operators for scattering problems 213 (1996) 313
- Storozhev, A.V., see Belikov, A.E. 213 (1996) 319
- Takeshima, M., see Oeda, Y. 213 (1996) 421
- Tao, Y., see Xie, X. 213 (1996) 133
- Tolosa, S. and J.A. Sansón, Molecular dynamics study of infinitely dilute aqueous solutions of small biological molecules. Calculation of the static and dynamic properties of formaldehyde 213 (1996) 203

- Tsurubuchi, S., see Motohashi, K. 213 (1996) 369
- Ukai, M., see Motohashi, K. 213 (1996) 369
- Vizoso, S. and B.M. Rode, Preferential solvation study: Solvation of sodium chloride in water-hydroxylamine mixtures 213 (1996) 77
- Waliszewska, G., see Kolodziejski, M. 213 (1996) 341
- Wallaart, H.L., see Porshnev, P.I. 213 (1996) 111
- Wang, H. and A.L. Cooksy, Calculations on ground and excited state potential energy surfaces of floppy free radicals: HC_4H_2 , HC_3NH , and HC_3O 213 (1996) 139
- Welker, M., G. Steinebrunner, J. Solca and H. Huber, Ab initio calculation of the intermolecular potential energy surface of $(\text{CO}_2)_2$ and first applications in simulations of fluid CO_2 213 (1996) 253
- Witschel, W., see Kohlmeyer, A. 213 (1996) 211
- Xie, X., Y. Tao, H. Cao and W. Duang, Ab initio study of unimolecular pyrolysis mechanisms of dithioformic acid 213 (1996) 133
- Yamaguchi, Y., see Matsushita, Y. 213 (1996) 413
- Yang, M.M., see Lossau, H. 213 (1996) 1
- Yencha, A.J., see Cormack, A.J. 213 (1996) 439
- Youvan, D.C., see Lossau, H. 213 (1996) 1
- Zhao, W., see Durig, J.R. 213 (1996) 165
- Zhou, L., see Durig, J.R. 213 (1996) 165
- Ziegeler, L., see Ruth, C. 213 (1996) 454



Subject index to volume 213

Methods

Theoretical

Group theory and algebras

- Dynamical symmetry in the vibrational overtone spectrum of monofluoroacetylene (HCCF),
E.S. Bernardes, Y.M.M. Hornos and J.E.M. Hornos 213 (1996) 17

Many body and quasiparticle approaches

- The ArClF Van der Waals complex as an example of how atoms inside a molecule interact
with those outside, F.Y. Naumkin 213 (1996) 33

Coupling schemes and perturbative treatments

- Spin–spin interactions in the reduced $[\text{Fe}_6\text{S}_6]^{5+}$ cluster, M. Czerwiński and J. Dąbrowski 213 (1996) 45

Equilibrium statistical mechanics

- A method to calculate the probability distribution for systems with large energy barriers, O.
Engkvist and G. Karlström 213 (1996) 63
Preferential solvation study: Solvation of sodium chloride in water–hydroxylamine mix-
tures, S. Vizoso and B.M. Rode 213 (1996) 77
Effect of ethanol addition upon the structure and the cooperativity of the water H bond
network, R. Lamanna and S. Cannistraro 213 (1996) 95

Non-equilibrium thermodynamic and hydrodynamic theories

- Modeling of optical pumping experiments in CO. I. Time-resolved experiments, P.I.
Porshnev, H.L. Wallaart, M.-Y. Perrin and J.-P. Martin 213 (1996) 111

Ab initio schemes for stationary properties

- Calculation of magnetizabilities using GIAO current density distributions, T.A. Keith 213 (1996) 123
Ab initio study of unimolecular pyrolysis mechanisms of dithioformic acid, X. Xie, Y. Tao,
H. Cao and W. Duang 213 (1996) 133
Calculations on ground and excited state potential energy surfaces of floppy free radicals:
 HC_4H_2 , HC_3NH , and HC_3O , H. Wang and A.L. Cooksy 213 (1996) 139
The use of locally dense basis sets in correlated NMR chemical shielding calculations, D.B.
Chesnut and E.F.C. Byrd 213 (1996) 153

- Correlation effects in the long-range coupling between acetylenic π -electrons in a series of α,ω -diethynyl[n]staffanes ($n = 1-5$), M. Braga 213 (1996) 159
- Conformational studies of cyclopropylcarbonyl fluoride from temperature dependent FT-IR spectra of xenon solutions, J.R. Durig, S. Shen, W. Zhao and L. Zhou 213 (1996) 165
- Conformational studies of propenoyl chloride in liquid xenon from temperature dependent FT-IR spectra, J.R. Durig, Y. Li and Y. Jin 213 (1996) 181
- An ab initio study of the potential energy surface in the S_1 state of 2-hydroxypyridine, A.L. Sobolewski and L. Adamowicz 213 (1996) 193
- Computational and simulation methods*
- Preferential solvation study: Solvation of sodium chloride in water-hydroxylamine mixtures, S. Vizoso and B.M. Rode 213 (1996) 77
- The use of locally dense basis sets in correlated NMR chemical shielding calculations, D.B. Chesnut and E.F.C. Byrd 213 (1996) 153
- Correlation effects in the long-range coupling between acetylenic π -electrons in a series of α,ω -diethynyl[n]staffanes ($n = 1-5$), M. Braga 213 (1996) 159
- Molecular dynamics study of infinitely dilute aqueous solutions of small biological molecules. Calculation of the static and dynamic properties of formaldehyde, S. Tolosa and J.A. Sansón 213 (1996) 203
- Molecular dynamics simulations of water/metal and water/vacuum interfaces with a polarizable water model, A. Kohlmeyer, W. Witschel and E. Spohr 213 (1996) 211
- Exploratory Pariser-Parr-Pople investigation of the static first hyperpolarizability of polymethineimine chains, D. Jacquemin, B. Champagne, J.-M. André and B. Kirtman 213 (1996) 217
- Optically pumped laser emission in K_2 involving rovibrational levels near the $B^1\Pi_u$ state dissociation limit, B.K. Clark, J.M. Standard, Z.J. Smolinski, D.P. Ripp and J.R. Fleming 213 (1996) 229
- On the sampling of microcanonical distribution for rotating triatomic molecules, I. Rosenblum, E.I. Dashevskaya, E.E. Nikitin and I. Oref 213 (1996) 243
- Ab initio calculation of the intermolecular potential energy surface of $(CO_2)_2$ and first applications in simulations of fluid CO_2 , M. Welker, G. Steinebrunner, J. Solca and H. Huber 213 (1996) 253
- Fast translational thermalization of extreme disequilibrium induced by cluster impact, T. Raz and R.D. Levine 213 (1996) 263
- Molecular dynamics and scattering theory*
- On the sampling of microcanonical distribution for rotating triatomic molecules, I. Rosenblum, E.I. Dashevskaya, E.E. Nikitin and I. Oref 213 (1996) 243
- Ab initio calculation of the intermolecular potential energy surface of $(CO_2)_2$ and first applications in simulations of fluid CO_2 , M. Welker, G. Steinebrunner, J. Solca and H. Huber 213 (1996) 253
- Fast translational thermalization of extreme disequilibrium induced by cluster impact, T. Raz and R.D. Levine 213 (1996) 263
- Second harmonic generation in partially ordered media and at interfaces: analysis of dynamical and orientational factors, D.L. Andrews and I.D. Hands 213 (1996) 277
- An IPA procedure for bound-continuum diatomic transition intensities, V.S. Ivanov and V.B. Sovkov 213 (1996) 295
- A critical analysis of the two-dimensional atom ellipsoid model to study rotational collisions, J.C. Belchior and J.P. Braga 213 (1996) 303

- A new method of calculating exponential operators for scattering problems, A.V. Storozhev 213 (1996) 313
 Rotational relaxation of nitrogen in helium, A.E. Belikov, R.G. Sharafutdinov and A.V. Storozhev 213 (1996) 319

Experimental

Magnetic resonances

- Effect of ethanol addition upon the structure and the cooperativity of the water H bond network, R. Lamanna and S. Cannistraro 213 (1996) 95

Infrared spectroscopy

- Conformational studies of cyclopropylcarbonyl fluoride from temperature dependent FT-IR spectra of xenon solutions, J.R. Durig, S. Shen, W. Zhao and L. Zhou 213 (1996) 165
 Conformational studies of propenoyl chloride in liquid xenon from temperature dependent FT-IR spectra, J.R. Durig, Y. Li and Y. Jin 213 (1996) 181
 IR induced isomerisation of HDO complexes: a method for the observation of FIR spectra of matrix isolated water complexes, A. Engdahl and B. Nelander 213 (1996) 333
 Vibrational dephasing in bromocyclohexane: how to separate contributions from different mechanisms, M. Kolodziejski, G. Waliszewska and H. Abramczyk 213 (1996) 341

Raman spectroscopy

- Vibrational dephasing in bromocyclohexane: how to separate contributions from different mechanisms, M. Kolodziejski, G. Waliszewska and H. Abramczyk 213 (1996) 341
 Influence of pressure on the ferroelectric phase transition in a symmetrical polymerizable diacetylene crystal DNP, J. Even, M. Bertault, A. Girard and Y. Délugeard 213 (1996) 357

Visible and UV spectroscopy

- Time-resolved spectroscopy of wild-type and mutant Green Fluorescent Proteins reveals excited state deprotonation consistent with fluorophore-protein interactions, H. Lossau, A. Kummer, R. Heinecke, F. Pöllinger-Dammer, C. Kompa, G. Bieser, T. Jonsson, C.M. Silva, M.M. Yang, D.C. Youvan and M.E. Michel-Beyerle 213 (1996) 1
 An ab initio study of the potential energy surface in the S_1 state of 2-hydroxypyridine, A.L. Sobolewski and L. Adamowicz 213 (1996) 193
 Interatomic potentials for XO^+ and B^31 states of intercombination cadmium line 326.1 nm broadened by Ar pressure, G.D. Roston, M.S. Helmi and T. Grycuk 213 (1996) 365
 Dissociative excitation of CH_4 by electron impact: Emission cross sections for the fragment species, K. Motohashi, H. Soshi, M. Ukai and S. Tsurubuchi 213 (1996) 369
 Photodissociation dynamics of $HN_3(DN_3) + h\nu \rightarrow H(D) + N_3$, M. Lock, K.-H. Gericke and F.J. Comes 213 (1996) 385

Fluorescence spectroscopy

- Time-resolved spectroscopy of wild-type and mutant Green Fluorescent Proteins reveals excited state deprotonation consistent with fluorophore-protein interactions, H. Lossau, A. Kummer, R. Heinecke, F. Pöllinger-Dammer, C. Kompa, G. Bieser, T. Jonsson, C.M. Silva, M.M. Yang, D.C. Youvan and M.E. Michel-Beyerle 213 (1996) 1
 An ab initio study of the potential energy surface in the S_1 state of 2-hydroxypyridine, A.L. Sobolewski and L. Adamowicz 213 (1996) 193

- Photodissociation dynamics of $\text{HN}_3(\text{DN}_3) + h\nu \rightarrow \text{H(D)} + \text{N}_3$, M. Lock, K.-H. Gericke and F.J. Comes 213 (1996) 385
- Laser-induced fluorescence excitation spectroscopy of jet-cooled tropolone-carbon monoxide van der Waals complexes, H.K. Sinha, V.J. MacKenzie and R.P. Steer 213 (1996) 397
- The photochemical reaction of excited acetophenone and benzaldehyde in the gas phase, Y. Matsushita, Y. Yamaguchi and T. Hikida 213 (1996) 413
- Exciton scattering, k selection rule, exciton bandwidth in pyrene microcrystallites, and lattice relaxation energy for the origin of V luminescence, Y. Oeda, O. Nishi, Y. Matsushima, K. Mizuno, A.H. Matsui, M. Michinomae, M. Takeshima and T. Goto 213 (1996) 421
- Triplet quantum yield determination by picosecond laser double-pulse fluorescence excitation, S. Reindl and A. Penzkofer 213 (1996) 429
- Photoelectron and Auger spectroscopy*
- High-resolution threshold photoelectron spectroscopy of molecular fluorine, A.J. Cormack, A.J. Yench, R.J. Donovan, K.P. Lawley, A. Hopkirk and G.C. King 213 (1996) 439
- Electron impact spectroscopy*
- Rotational relaxation of nitrogen in helium, A.E. Belikov, R.G. Sharafutdinov and A.V. Storozhev 213 (1996) 319
- Laser methods*
- Optically pumped laser emission in K_2 involving rovibrational levels near the $\text{B}^1\Pi_u$ state dissociation limit, B.K. Clark, J.M. Standard, Z.J. Smolinski, D.P. Ripp and J.R. Fleming 213 (1996) 229
- IR induced isomerisation of HDO complexes: a method for the observation of FIR spectra of matrix isolated water complexes, A. Engdahl and B. Nelander 213 (1996) 333
- Picosecond spectroscopy*
- Triplet quantum yield determination by picosecond laser double-pulse fluorescence excitation, S. Reindl and A. Penzkofer 213 (1996) 429
- Non-linear optical spectroscopy*
- Triplet quantum yield determination by picosecond laser double-pulse fluorescence excitation, S. Reindl and A. Penzkofer 213 (1996) 429
- Synchrotron spectroscopies*
- High-resolution threshold photoelectron spectroscopy of molecular fluorine, A.J. Cormack, A.J. Yench, R.J. Donovan, K.P. Lawley, A. Hopkirk and G.C. King 213 (1996) 439
- Coherent optical spectroscopy*
- Optically pumped laser emission in K_2 involving rovibrational levels near the $\text{B}^1\Pi_u$ state dissociation limit, B.K. Clark, J.M. Standard, Z.J. Smolinski, D.P. Ripp and J.R. Fleming 213 (1996) 229
- Time-resolved experiments*
- Modeling of optical pumping experiments in CO. I. Time-resolved experiments, P.I. Porshnev, H.L. Wallaart, M.-Y. Perrin and J.-P. Martin 213 (1996) 111

- Positronium dynamics in aqueous solutions of ionic surfactants, G. Consolati and F. Quasso 213 (1996) 449
- Influence of the molecular environment on the hyperfine interaction of ^{111}Cd ions in gaseous radioactive indium halides, C. Ruth, M. Gründel, I. Eschrich, L. Ziegeler and I. Borchert 213 (1996) 454

Light scattering

- Analysis of polarization effects in time-dependent Rayleigh light scattering by optically active molecules, K. Knast 213 (1996) 465

Measurement of macroscopic variables

- Electric permittivity in the one- and two-phase region of 1-nitropropane-hexadecane near-critical solution, M. Paluch, P. Haldas, S.J. Rzoska and T. Schimpel 213 (1996) 483

Objects

Bulk systems

Gases

- Modeling of optical pumping experiments in CO. I. Time-resolved experiments, P.I. Porshnev, H.L. Wallaart, M.-Y. Perrin and J.-P. Martin 213 (1996) 111
- A new method of calculating exponential operators for scattering problems, A.V. Storozhev 213 (1996) 313
- Interatomic potentials for $X0^+$ and B^31 states of intercombination cadmium line 326.1 nm broadened by Ar pressure, G.D. Roston, M.S. Helmi and T. Grycuk 213 (1996) 365
- The photochemical reaction of excited acetophenone and benzaldehyde in the gas phase, Y. Matsushita, Y. Yamaguchi and T. Hikida 213 (1996) 413

Liquids neat

- A method to calculate the probability distribution for systems with large energy barriers, O. Engkvist and G. Karlström 213 (1996) 63
- Analysis of polarization effects in time-dependent Rayleigh light scattering by optically active molecules, K. Knast 213 (1996) 465

Liquid mixtures and solutions

- A method to calculate the probability distribution for systems with large energy barriers, O. Engkvist and G. Karlström 213 (1996) 63
- Preferential solvation study: Solvation of sodium chloride in water-hydroxylamine mixtures, S. Vizoso and B.M. Rode 213 (1996) 77
- Effect of ethanol addition upon the structure and the cooperativity of the water H bond network, R. Lamanna and S. Cannistraro 213 (1996) 95
- Conformational studies of cyclopropylcarbonyl fluoride from temperature dependent FT-IR spectra of xenon solutions, J.R. Durig, S. Shen, W. Zhao and L. Zhou 213 (1996) 165
- Conformational studies of propenoyl chloride in liquid xenon from temperature dependent FT-IR spectra, J.R. Durig, Y. Li and Y. Jin 213 (1996) 181
- Molecular dynamics study of infinitely dilute aqueous solutions of small biological molecules. Calculation of the static and dynamic properties of formaldehyde, S. Tolosa and J.A. Sansón 213 (1996) 203

- Vibrational dephasing in bromocyclohexane: how to separate contributions from different mechanisms, M. Kolodziejewski, G. Waliszewska and H. Abramczyk 213 (1996) 341
- Positronium dynamics in aqueous solutions of ionic surfactants, G. Consolati and F. Quasso 213 (1996) 449
- Electric permittivity in the one- and two-phase region of 1-nitropropane-hexadecane near-critical solution, M. Paluch, P. Habdas, S.J. Rzoska and T. Schimpel 213 (1996) 483

Crystals

-neat

- Exciton scattering, k selection rule, exciton bandwidth in pyrene microcrystallites, and lattice relaxation energy for the origin of V luminescence, Y. Oeda, O. Nishi, Y. Matsushima, K. Mizuno, A.H. Matsui, M. Michinomae, M. Takeshima and T. Goto 213 (1996) 421

Polymers

- Second harmonic generation in partially ordered media and at interfaces: analysis of dynamical and orientational factors, D.L. Andrews and I.D. Hands 213 (1996) 277

Thin films

- Molecular dynamics simulations of water/metal and water/vacuum interfaces with a polarizable water model, A. Kohlmeyer, W. Witschel and E. Spohr 213 (1996) 211

Surfaces

- Molecular dynamics simulations of water/metal and water/vacuum interfaces with a polarizable water model, A. Kohlmeyer, W. Witschel and E. Spohr 213 (1996) 211
- Second harmonic generation in partially ordered media and at interfaces: analysis of dynamical and orientational factors, D.L. Andrews and I.D. Hands 213 (1996) 277

Dielectrics

- Electric permittivity in the one- and two-phase region of 1-nitropropane-hexadecane near-critical solution, M. Paluch, P. Habdas, S.J. Rzoska and T. Schimpel 213 (1996) 483

Microscopic systems

Molecules (neutral and ionic)

- Calculation of magnetizabilities using GIAO current density distributions, T.A. Keith 213 (1996) 123
- Ab initio study of unimolecular pyrolysis mechanisms of dithioformic acid, X. Xie, Y. Tao, H. Cao and W. Duang 213 (1996) 133
- An ab initio study of the potential energy surface in the S_1 state of 2-hydroxypyridine, A.L. Sobolewski and L. Adamowicz 213 (1996) 193
- On the sampling of microcanonical distribution for rotating triatomic molecules, I. Rosenblum, E.I. Dashevskaya, E.E. Nikitin and I. Oref 213 (1996) 243
- A critical analysis of the two-dimensional atom ellipsoid model to study rotational collisions, J.C. Belchior and J.P. Braga 213 (1996) 303
- A new method of calculating exponential operators for scattering problems, A.V. Storozhev 213 (1996) 313
- Dissociative excitation of CH_4 by electron impact: Emission cross sections for the fragment species, K. Motohashi, H. Soshi, M. Ukai and S. Tsurubuchi 213 (1996) 369
- Photodissociation dynamics of $\text{HN}_3(\text{DN}_3) + h\nu \rightarrow \text{H(D)} + \text{N}_3$, M. Lock, K.-H. Gericke and F.J. Comes 213 (1996) 385

- High-resolution threshold photoelectron spectroscopy of molecular fluorine, A.J. Cormack, A.J. Yench, R.J. Donovan, K.P. Lawley, A. Hopkirk and G.C. King 213 (1996) 439
- diatomic*
- Optically pumped laser emission in K_2 involving rovibrational levels near the $B^1\Pi_u$ state dissociation limit, B.K. Clark, J.M. Standard, Z.J. Smolinski, D.P. Ripp and J.R. Fleming 213 (1996) 229
- An IPA procedure for bound-continuum diatomic transition intensities, V.S. Ivanov and V.B. Sovkov 213 (1996) 295
- Rotational relaxation of nitrogen in helium, A.E. Belikov, R.G. Sharafutdinov and A.V. Storozhev 213 (1996) 319
- Interatomic potentials for XO^+ and B^31 states of intercombination cadmium line 326.1 nm broadened by Ar pressure, G.D. Roston, M.S. Helmi and T. Grycuk 213 (1996) 365
- High-resolution threshold photoelectron spectroscopy of molecular fluorine, A.J. Cormack, A.J. Yench, R.J. Donovan, K.P. Lawley, A. Hopkirk and G.C. King 213 (1996) 439
- Influence of the molecular environment on the hyperfine interaction of ^{111}Cd ions in gaseous radioactive indium halides, C. Ruth, M. Gründel, I. Eschrich, L. Ziegeler and I. Borchert 213 (1996) 454
- small polyatomics*
- Dynamical symmetry in the vibrational overtone spectrum of monofluoroacetylene (HCCF), E.S. Bernardes, Y.M.M. Hornos and J.E.M. Hornos 213 (1996) 17
- The ArClF Van der Waals complex as an example of how atoms inside a molecule interact with those outside, F.Y. Naumkin 213 (1996) 33
- The use of locally dense basis sets in correlated NMR chemical shielding calculations, D.B. Chesnut and E.F.C. Byrd 213 (1996) 153
- A critical analysis of the two-dimensional atom ellipsoid model to study rotational collisions, J.C. Belchior and J.P. Braga 213 (1996) 303
- Dissociative excitation of CH_4 by electron impact: Emission cross sections for the fragment species, K. Motohashi, H. Soshi, M. Ukai and S. Tsurubuchi 213 (1996) 369
- aromatics*
- Triplet quantum yield determination by picosecond laser double-pulse fluorescence excitation, S. Reindl and A. Penzkofer 213 (1996) 429
- polymeric and biological*
- Exploratory Pariser–Parr–Pople investigation of the static first hyperpolarizability of polymethineimine chains, D. Jacquemin, B. Champagne, J.-M. André and B. Kirtman 213 (1996) 217
- Influence of pressure on the ferroelectric phase transition in a symmetrical polymerizable diacetylene crystal DNP, J. Even, M. Bertault, A. Girard and Y. Délugeard 213 (1996) 357
- Molecular aggregates*
- Preferential solvation study: Solvation of sodium chloride in water–hydroxylamine mixtures, S. Vizoso and B.M. Rode 213 (1996) 77
- IR induced isomerisation of HDO complexes: a method for the observation of FIR spectra of matrix isolated water complexes, A. Engdahl and B. Nelander 213 (1996) 333

- Positronium dynamics in aqueous solutions of ionic surfactants, G. Consolati and F. Quasso 213 (1996) 449
- dimers*
- Ab initio calculation of the intermolecular potential energy surface of $(\text{CO}_2)_2$ and first applications in simulations of fluid CO_2 , M. Welker, G. Steinebrunner, J. Solca and H. Huber 213 (1996) 253
- Influence of the molecular environment on the hyperfine interaction of ^{111}Cd ions in gaseous radioactive indium halides, C. Ruth, M. Gründel, I. Eschrich, L. Ziegeler and I. Borchert 213 (1996) 454
- van der Waals molecules*
- The ArClF Van der Waals complex as an example of how atoms inside a molecule interact with those outside, F.Y. Naumkin 213 (1996) 33
- Laser-induced fluorescence excitation spectroscopy of jet-cooled tropolone-carbon monoxide van der Waals complexes, H.K. Sinha, V.J. MacKenzie and R.P. Steer 213 (1996) 397
- clusters*
- Spin-spin interactions in the reduced $[\text{Fe}_6\text{S}_6]^{5+}$ cluster, M. Czerwiński and J. Dąbrowski 213 (1996) 45
- Fast translational thermalization of extreme disequilibrium induced by cluster impact, T. Raz and R.D. Levine 213 (1996) 263
- complexes*
- Laser-induced fluorescence excitation spectroscopy of jet-cooled tropolone-carbon monoxide van der Waals complexes, H.K. Sinha, V.J. MacKenzie and R.P. Steer 213 (1996) 397
- Free radicals (including hydronium and muonium)*
- Calculations on ground and excited state potential energy surfaces of floppy free radicals: HC_4H_2 , HC_3NH , and HC_3O , H. Wang and A.L. Cooksy 213 (1996) 139
- Quasiparticles (including excitons)*
- Exciton scattering, k selection rule, exciton bandwidth in pyrene microcrystallites, and lattice relaxation energy for the origin of V luminescence, Y. Oeda, O. Nishi, Y. Matsushima, K. Mizuno, A.H. Matsui, M. Michinomae, M. Takeshima and T. Goto 213 (1996) 421

Phenomena

Molecular structure

- Dynamical symmetry in the vibrational overtone spectrum of monofluoroacetylene (HCCF), E.S. Bernardes, Y.M.M. Hornos and J.E.M. Hornos 213 (1996) 17
- The ArClF Van der Waals complex as an example of how atoms inside a molecule interact with those outside, F.Y. Naumkin 213 (1996) 33
- Calculations on ground and excited state potential energy surfaces of floppy free radicals: HC_4H_2 , HC_3NH , and HC_3O , H. Wang and A.L. Cooksy 213 (1996) 139

Vibrations and rotations of molecules

- Dynamical symmetry in the vibrational overtone spectrum of monofluoroacetylene (HCCF), E.S. Bernardes, Y.M.M. Hornos and J.E.M. Hornos 213 (1996) 17
- Conformational studies of cyclopropylcarbonyl fluoride from temperature dependent FT-IR spectra of xenon solutions, J.R. Durig, S. Shen, W. Zhao and L. Zhou 213 (1996) 165
- Conformational studies of propenoyl chloride in liquid xenon from temperature dependent FT-IR spectra, J.R. Durig, Y. Li and Y. Jin 213 (1996) 181
- On the sampling of microcanonical distribution for rotating triatomic molecules, I. Rosenblum, E.I. Dashevskaya, E.E. Nikitin and I. Oref 213 (1996) 243
- IR induced isomerisation of HDO complexes: a method for the observation of FIR spectra of matrix isolated water complexes, A. Engdahl and B. Nelander 213 (1996) 333
- Vibrational dephasing in bromocyclohexane: how to separate contributions from different mechanisms, M. Kolodziejcki, G. Waliszewska and H. Abramczyk 213 (1996) 341

Electronic structure and states

- Calculations on ground and excited state potential energy surfaces of floppy free radicals: HC_4H_2 , HC_3NH , and HC_3O , H. Wang and A.L. Cooksy 213 (1996) 139
- The use of locally dense basis sets in correlated NMR chemical shielding calculations, D.B. Chesnut and E.F.C. Byrd 213 (1996) 153
- Dissociative excitation of CH_4 by electron impact: Emission cross sections for the fragment species, K. Motohashi, H. Soshi, M. Ukai and S. Tsurubuchi 213 (1996) 369

Electric and magnetic properties

- Spin-spin interactions in the reduced $[\text{Fe}_6\text{S}_6]^{5+}$ cluster, M. Czerwiński and J. Dąbrowski 213 (1996) 45
- Calculation of magnetizabilities using GIAO current density distributions, T.A. Keith 213 (1996) 123
- The use of locally dense basis sets in correlated NMR chemical shielding calculations, D.B. Chesnut and E.F.C. Byrd 213 (1996) 153

Optical activity

- Analysis of polarization effects in time-dependent Rayleigh light scattering by optically active molecules, K. Knast 213 (1996) 465

Molecular interactions

- The ArCIF Van der Waals complex as an example of how atoms inside a molecule interact with those outside, F.Y. Naumkin 213 (1996) 33
- Molecular dynamics study of infinitely dilute aqueous solutions of small biological molecules. Calculation of the static and dynamic properties of formaldehyde, S. Tolosa and J.A. Sansón 213 (1996) 203
- A new method of calculating exponential operators for scattering problems, A.V. Storozhev 213 (1996) 313
- Rotational relaxation of nitrogen in helium, A.E. Belikov, R.G. Sharafutdinov and A.V. Storozhev 213 (1996) 319
- IR induced isomerisation of HDO complexes: a method for the observation of FIR spectra of matrix isolated water complexes, A. Engdahl and B. Nelander 213 (1996) 333
- Vibrational dephasing in bromocyclohexane: how to separate contributions from different mechanisms, M. Kolodziejcki, G. Waliszewska and H. Abramczyk 213 (1996) 341
- Influence of pressure on the ferroelectric phase transition in a symmetrical polymerizable diacetylene crystal DNP, J. Even, M. Bertault, A. Girard and Y. Délugeard 213 (1996) 357

- The photochemical reaction of excited acetophenone and benzaldehyde in the gas phase, Y. Matsushita, Y. Yamaguchi and T. Hikida 213 (1996) 413
- Spectral bandshapes and intensities*
- Conformational studies of cyclopropylcarbonyl fluoride from temperature dependent FT-IR spectra of xenon solutions, J.R. Durig, S. Shen, W. Zhao and L. Zhou 213 (1996) 165
- Conformational studies of propenoyl chloride in liquid xenon from temperature dependent FT-IR spectra, J.R. Durig, Y. Li and Y. Jin 213 (1996) 181
- Interatomic potentials for XO^+ and $B^3\Gamma$ states of intercombination cadmium line 326.1 nm broadened by Ar pressure, G.D. Roston, M.S. Helmi and T. Gryczuk 213 (1996) 365
- Exciton scattering, k selection rule, exciton bandwidth in pyrene microcrystallites, and lattice relaxation energy for the origin of V luminescence, Y. Oeda, O. Nishi, Y. Matsushima, K. Mizuno, A.H. Matsui, M. Michinomae, M. Takeshima and T. Goto 213 (1996) 421
- Coupling of electronic and nuclear motion*
- Influence of the molecular environment on the hyperfine interaction of ^{111}Cd ions in gaseous radioactive indium halides, C. Ruth, M. Gründel, I. Eschrich, L. Ziegeler and I. Borchert 213 (1996) 454
- Energy transfer processes*
- Modeling of optical pumping experiments in CO. I. Time-resolved experiments, P.I. Porshnev, H.L. Wallaart, M.-Y. Perrin and J.-P. Martin 213 (1996) 111
- Fast translational thermalization of extreme disequilibrium induced by cluster impact, T. Raz and R.D. Levine 213 (1996) 263
- A critical analysis of the two-dimensional atom ellipsoid model to study rotational collisions, J.C. Belchior and J.P. Braga 213 (1996) 303
- Rotational relaxation of nitrogen in helium, A.E. Belikov, R.G. Sharafutdinov and A.V. Storozhev 213 (1996) 319
- Molecular photophysical processes*
- Time-resolved spectroscopy of wild-type and mutant Green Fluorescent Proteins reveals excited state deprotonation consistent with fluorophore-protein interactions, H. Lossau, A. Kummer, R. Heinecke, F. Pöllinger-Dammer, C. Kompa, G. Bieser, T. Jonsson, C.M. Silva, M.M. Yang, D.C. Youvan and M.E. Michel-Beyerle 213 (1996) 1
- Triplet quantum yield determination by picosecond laser double-pulse fluorescence excitation, S. Reindl and A. Penzkofer 213 (1996) 429
- Intramolecular dynamics*
- Calculations on ground and excited state potential energy surfaces of floppy free radicals: HC_4H_2 , HC_3NH , and HC_3O , H. Wang and A.L. Cooksy 213 (1996) 139
- Fast translational thermalization of extreme disequilibrium induced by cluster impact, T. Raz and R.D. Levine 213 (1996) 263
- An IPA procedure for bound-continuum diatomic transition intensities, V.S. Ivanov and V.B. Sovkov 213 (1996) 295
- vibrational energy redistribution (including vibrational dissociation)*
- Modeling of optical pumping experiments in CO. I. Time-resolved experiments, P.I. Porshnev, H.L. Wallaart, M.-Y. Perrin and J.-P. Martin 213 (1996) 111

Luminescence spectra, yields and lifetimes

- Time-resolved spectroscopy of wild-type and mutant Green Fluorescent Proteins reveals excited state deprotonation consistent with fluorophore-protein interactions, H. Lossau, A. Kummer, R. Heinecke, F. Pöllinger-Dammer, C. Kompa, G. Bieser, T. Jonsson, C.M. Silva, M.M. Yang, D.C. Youvan and M.E. Michel-Beyerle 213 (1996) 1

Non-linear responses (including optical)

- Exploratory Pariser-Parr-Pople investigation of the static first hyperpolarizability of polymethineimine chains, D. Jacquemin, B. Champagne, J.-M. André and B. Kirtman 213 (1996) 217
- Second harmonic generation in partially ordered media and at interfaces: analysis of dynamical and orientational factors, D.L. Andrews and I.D. Hands 213 (1996) 277

Reactions (including dissociation)

- Ab initio study of unimolecular pyrolysis mechanisms of dithioformic acid, X. Xie, Y. Tao, H. Cao and W. Duang 213 (1996) 133

-gas phase

- Ab initio study of unimolecular pyrolysis mechanisms of dithioformic acid, X. Xie, Y. Tao, H. Cao and W. Duang 213 (1996) 133
- The photochemical reaction of excited acetophenone and benzaldehyde in the gas phase, Y. Matsushita, Y. Yamaguchi and T. Hikida 213 (1996) 413

-photochemical

- Photodissociation dynamics of $\text{HN}_3(\text{DN}_3) + h\nu \rightarrow \text{H(D)} + \text{N}_3$, M. Lock, K.-H. Gericke and F.J. Comes 213 (1996) 385

Tunnelling

- Laser-induced fluorescence excitation spectroscopy of jet-cooled tropolone-carbon monoxide van der Waals complexes, H.K. Sinha, V.J. MacKenzie and R.P. Steer 213 (1996) 397

Electron transfer

- Spin-spin interactions in the reduced $[\text{Fe}_6\text{S}_6]^{5+}$ cluster, M. Czerwiński and J. Dąbrowski 213 (1996) 45
- Correlation effects in the long-range coupling between acetylenic π -electrons in a series of α,ω -diethynyl[n]staffanes ($n = 1-5$), M. Braga 213 (1996) 159
- The photochemical reaction of excited acetophenone and benzaldehyde in the gas phase, Y. Matsushita, Y. Yamaguchi and T. Hikida 213 (1996) 413
- Influence of the molecular environment on the hyperfine interaction of ^{111}Cd ions in gaseous radioactive indium halides, C. Ruth, M. Gründel, I. Eschrich, L. Ziegeler and I. Borchert 213 (1996) 454

Positron annihilation

- Positronium dynamics in aqueous solutions of ionic surfactants, G. Consolati and F. Quasso 213 (1996) 449

Ionization (including Rydberg states)

- High-resolution threshold photoelectron spectroscopy of molecular fluorine, A.J. Cormack, A.J. Yench, R.J. Donovan, K.P. Lawley, A. Hopkirk and G.C. King 213 (1996) 439

Molecular motion (including diffusive)

- Second harmonic generation in partially ordered media and at interfaces: analysis of dynamical and orientational factors, D.L. Andrews and I.D. Hands 213 (1996) 277

- Analysis of polarization effects in time-dependent Rayleigh light scattering by optically active molecules, K. Knast 213 (1996) 465
- Surface effects and catalysis*
- Exciton scattering, *k* selection rule, exciton bandwidth in pyrene microcrystallites, and lattice relaxation energy for the origin of V luminescence, Y. Oeda, O. Nishi, Y. Matsushima, K. Mizuno, A.H. Matsui, M. Michinomae, M. Takeshima and T. Goto 213 (1996) 421
- Thermodynamic and transport properties*
- Effect of ethanol addition upon the structure and the cooperativity of the water H bond network, R. Lamanna and S. Cannistraro 213 (1996) 95
- Ab initio calculation of the intermolecular potential energy surface of (CO₂)₂ and first applications in simulations of fluid CO₂, M. Welker, G. Steinebrunner, J. Solca and H. Huber 213 (1996) 253
- Structure of solids and liquids*
- A method to calculate the probability distribution for systems with large energy barriers, O. Engkvist and G. Karlström 213 (1996) 63
- Molecular dynamics simulations of water/metal and water/vacuum interfaces with a polarizable water model, A. Kohlmeyer, W. Witschel and E. Spohr 213 (1996) 211
- Ab initio calculation of the intermolecular potential energy surface of (CO₂)₂ and first applications in simulations of fluid CO₂, M. Welker, G. Steinebrunner, J. Solca and H. Huber 213 (1996) 253
- Critical phenomena*
- Electric permittivity in the one- and two-phase region of 1-nitropropane-hexadecane near-critical solution, M. Paluch, P. Habdas, S.J. Rzoska and T. Schimpel 213 (1996) 483
- Phase transitions*
- Influence of pressure on the ferroelectric phase transition in a symmetrical polymerizable diacetylene crystal DNP, J. Even, M. Bertault, A. Girard and Y. Délugeard 213 (1996) 357